MO 13: Cold Molecules (joint session MO/Q)

Time: Wednesday 14:00–15:15 Location: f102

MO 13.1 Wed 14:00 f102

Optical pumping of metastable helium: state purification and spin-state selection — •J. Guan, T. Sixt, A. Tsoukala, F. Stienkemeier, and K. Dulitz — Institute of Physics, University of Freiburg, Herman-Herder-Str.3, 79104 Freiburg, Germany

Discharge and electron-impact excitation lead to the production of metastable helium atoms in two metastable states, 2^3S_1 and 2^1S_0. However, many applications require purified beams containing only one of these species. For atom magnetometers and spin-controlled collisions, even magnetic quantum state selection is required.

Recently, we have successfully applied optical quenching via the $4^1P_1 \leftarrow 2^1S_0$ transition at 397 nm to fully deplete the 2^1S_0 population in a ^{4}He gas beam.[1] Equipped with a tunable laser at 1083 nm for excitation of $2^3S_1 \rightarrow 2^3P$ transitions, we continue to make progresses on preparing the spin-labelled 2^3S_1 state after optical quenching. In this talk, I will show our results on the optical quenching of He (2^1S_0) and on the optical pumping of He (2^3S_1). The spin-controlled metastable He atoms (2^3S_1, $m_J = 1$, 0 or -1) are an ideal source for studying cold and controlled reactive collisions and I will outline possible experiments using this setup.

Reference: 1. Guan et al., Phys. Rev. Appl. 11, 054073 (2019).

MO 13.2 Wed 14:15 f102

The diatomic molecular spectroscopy database for laser cooling and trapping — •Xiangyue Liu, Stefan Truppe, Gerard Meijer, and Jesus Perez-Rios — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Convenient access to the spectroscopic constants of molecules is essential for the screening of potential candidates for laser cooling and trapping techniques. To this end, we present a user-friendly database-driven website that provides the ground and excited states spectroscopy constants of polar diatomic molecules, implemented with Linux, Apache, MySQL, and PHP (LAMP) on the back end. The Franck-Condon factors, which directly determine the transition probabilities between two vibrational states, are directly calculated from the spectroscopic constants. In this website, the user can either search for the spectroscopic constants from the web page user interface or access freely to the data from the application programming interface (API). In the API, the data is given in in lightweight data-interchange formats, including JSON and CSV. The user, after registration, is also allowed to contribute to the database. We believe that this database may advance the research in molecular spectroscopy and, ultimately, in ultracold molecules.

MO 13.3 Wed 14:30 f102

Suppression of Penning ionization by orbital angular momentum conservation — •Tobias Sixt, Jiwen Guan, Jonas Grzesiak, Markus Debatin, Frank Stienkemeier, and Katrin Dulitz — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg im Breisgau, Germany

The efficient suppression of Penning-ionizing collisions is a stringent requirement to achieve quantum degeneracy in metastable rare gases. In our experiment, we study quantum-state-controlled Penning collisions between laser-cooled lithium atoms (Li) and metastable helium atoms (He*) to investigate new ways of controlling the outcome of Penning-ionizing collisions.

In this contribution, we report on the efficient suppression of He*-Li Penning ionization by laser excitation of the Li atoms. The results illustrate that not only the electron spin, but also Λ - the projection of the total molecular orbital angular momentum along the internuclear axis - is conserved during the ionization process. Our findings suggest that Λ conservation can be used as a more general means of reaction control, for example, to improve schemes for the simultaneous laser cooling and trapping of He* and alkali atoms.

MO 13.4 Wed 14:45 f102

Line shape investigation of the electronic origin of phthalocyanines, porphyrins and their clusters with H_2O I: Helium nanodroplet studies — •Johannes Fischer, Florian Schlaghaufer, and Alkwin Slenczka — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93053 Regensburg, Germany

Despite vanishing viscosity the spectral shape of the zero phonon line at the electronic origin of molecules embedded into superfluid helium nanodroplets does not reveal the band system of a free rotor. According to previous investigations, helium induced inhomogeneous line broadening dominates the experimentally observed optical line shape. To decipher pure molecular and helium induced contributions the line shapes of various organic compounds and their clusters with H_2O were recorded by means of electronic spectroscopy as well as electronic Stark spectroscopy. In order to learn about the dopant species its spectroscopic response must be separated from the helium induced spectral features. We present electronic spectra and Stark-spectra of phthalocyanine-H_2O clusters, dipolar chloroaluminiumphthalocyanine, and of chloroaluminiumphthalocyanine-H_2O clusters. Thereby we observe field induced optical anisotropy and spectral changes of the line shape. A final analysis requires in addition high-level *ab initio* calculations for the corresponding isolated species [1]. Moreover, the helium droplet work is accompanied by corresponding investigations in the gas phase, which are subject of a follow up talk (F. Schlaghaufer).

[1] J. Fischer et al., *J. Phys. Chem.*, **123**, 10057, (2019).

MO 13.5 Wed 15:00 f102

Line shape investigation of the electronic origin of phthalocyanines, porphyrins and their clusters with H_2O II: gas phase studies — •Florian Schlaghaufer, Johannes Fischer, and Alkwin Slenczka — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93053 Regensburg, Germany

The spectral shape of the zero-phonon-line in the electronic and Stark spectra of organic molecules such as phthalocyanines [1] and porphine [2] and their clusters with small molecules (e.g. H_2O) recorded in superfluid helium nanodroplets is determined by pure molecular contributions and the influence of the helium environment. As discussed in an accompanying talk (J. Fischer), the analysis of such line shapes is not straightforward. Therefore, corresponding gas phase studies are essential for dissecting helium induced spectral features from molecular rotor fingerprints. The observed rotational band shapes of jet cooled molecules and associated simulations give insight into the structure and polarity of the molecular systems for both the ground and the electronically excited state. By means of a rule of thumb for transition from gas phase to helium droplet conditions we compare these simulations with experimental spectra measured in helium droplets. Mismatches reveal the influence of helium induced contributions to the line shapes. Ultimately, this project heads for a better understanding of microsolvation and the dynamics of electronic excitation of molecules inside superfluid helium nanodroplets.

[1] J. Chem. Phys. 2018, 148, 144301.
[2] J. Chem. Phys. 2018, 149, 244306.